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Experimental and numerical investigation of explosive behavior of syngas/air mixtures

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ABSTRACT

In this study, the explosive behavior of syngas/air mixtures was investigated numerically in a 3-D cylindrical geometric model, using ANSYS Fluent. A chamber with the same dimensions as the geometry in the simulation was used to investigate the explosion process experimentally. The outcome was in good agreement with experimental results for most equivalence ratios at atmospheric pressure, while discrepancies were observed for very rich mixtures ($\phi > 2.0$) and at elevated pressure conditions. Both the experimental and simulated results showed that for syngas/air mixture, the maximum explosion pressure increased from lean ($\phi = 0.8$) to an equivalence ratio of 1.2, then decreased significantly with richer mixtures, indicating that maximum explosion pressure occurred at the equivalence ratio of 1.2, while explosion time was shortest at an equivalence ratio of 1.6. Increasing H_2 content in the fuel blends significantly raised laminar burning velocity and shortened the explosion time, thereby increasing the maximum rate of pressure rise and deflagration index. Normalized peak pressure, the maximum rate of pressure rise and the deflagration index were sensitive to the initial pressure of the mixture, showing that they increased significantly with increased initial pressure.

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Introduction

Conventional fossil fuels such as oil, natural gas, and coal still supply about 80% of the world's energy [1], but due to their limited availability they are expected to be depleted within 40 or 50 years. In the meantime, byproducts from fossil fuel combustion are a major source of environmental problems––the greenhouse effect, ozone depletion and climate change. In this context, syngas has emerged as the likely candidate for greener energy conversion since it possesses numerous advantages in stationary power generation [2–4]. Syngas is formed in a gasification process of coal, biomass, organic wastes and refinery residuals, and it primarily contains hydrogen and carbon monoxide. Depending on the fuel sources and/or processing techniques used to produce it, syngas can also contain nitrogen, carbon dioxide, water, methane and higher-order hydrocarbons [5,6].

In transportation, storage and fuel usage, explosion is a serious hazard that causes injury and damage to its surroundings. When such an explosion takes place in a closed chamber, without proper venting or suppressing devices, it can damage the combustion chamber. To prevent such incidents, it is necessary to understand fuel explosion behavior and its proper use.

Among the combustion characteristics being investigated, maximum rate of pressure rise during explosion in a closed chamber, $(dP/dt)_{max}$, and the deflagration index, K_G, are the most important explosion characteristics of premixture combustion. Because $(dP/dt)_{max}$ depends on both the mixture properties (mixture composition, initial pressure and initial temperature) and the volume of the combustion chamber, V, it is normalized with respect to the chamber volume and according to the cubic root law [7–9] to obtain a deflagration index that is an intrinsic property of the premixture, so that K_G is independent of the combustion chamber volume,

$$K_G = (dP/dt)_{max} \times V^{1/3} \quad (1)$$

The deflagration index is used to evaluate the explosive consequence of a mixture [8]. Other fundamental parameters that characterize the explosion, and will be evaluated here, include maximum explosion pressure, or the highest pressure attained during the explosion, P_{max}, and the explosion time, t_c, defined as the interval of time between ignition and the moment when maximum pressure is reached.

Investigations of explosion characteristics of syngas/air mixtures have reported that the flame's maximum explosion pressure decreased with the addition of H_2O, due to a decrease in adiabatic flame temperature [10]. It is interesting that normalized explosion pressure increased while normalized adiabatic explosion pressure decreased with a higher CO/H_2 ratio [10]. The explosion limits of $H_2/CO/O_2$ mixtures were analyzed computationally and theoretically, results showed that the limits changed dramatically with just a small amount of added hydrogen. With the further addition of H_2, limits evolved towards those of pure H_2 flame [11]. Moreover, a previous study by this group [12] showed that, with the addition of methane or propane to a syngas/air mixture, both maximum pressure and time of the explosion increased linearly with the hydrocarbon concentration; however, the maximum rate of pressure rise decreased in a nonlinear manner. When the syngas/air mixture was diluted with helium or nitrogen, the maximum pressure was found to decrease while the explosion time increased linearly with the diluent concentration. The maximum rate of pressure rise was thus significantly reduced [12].

In a computational study of the explosion characteristics of methane, hydrogen, and their mixtures [13], it was stated that the linear relationship between $(dP/dt)_{max}$ and initial pressure was not accurate for methane fuel, but instead, the simulated rate of pressure rise was proportional to the initial pressure to the power of 0.7 [13]. (It is noted that a code named A-SURF, developed by these authors, was employed in their work.)

Computational fluid dynamics (CFD) coupled to chemical mechanism has been revealed as a numerical simulation technique to predict combustion performance resulting from physical and chemical processes of a flame. Among commercial softwares, ANSYS Fluent has been widely used to solve complex compressible and non-compressible fluid flows, including simulation of the combustion process in a closed chamber [14–16]. The effect of blockage ratio on the flame acceleration process and the flame-vortex mechanism in an obstructed chamber was studied [14]. Flame propagation through three obstacle-blockage ratio configurations was simulated, showing that the peak of flame tip speed and pressure growth rate increased with the blockage ratio [14]. A 2-D geometry with global one-step reaction mechanism for methane combustion was employed to investigate the propagation velocity of a flame kernel in horizontal tubes with a wide range of tube diameters [15]. It was reported that the spark model was suitable to simulate a flame propagating with the detonation speed, but did not help in the study of deflagration combustion. Results also showed that, for a given mixture condition, the larger tube diameter led to a greater uniform burning velocity; the maximum burning velocity in all cases occurring near stoichiometric conditions [15]. An explosion was carried out in a large-scale tank to investigate the influence of tank capacity, height-to-diameter ratio, roof form, flammable gas species and height of underlying oil level on the magnitude and distribution of an internal explosion loading on the tank wall [16].

The objective of this study is to experimentally and numerically investigate the explosion behaviors of syngas/air mixtures at various equivalence ratios, H_2:CO ratios, and initial pressures, using ANSYS Fluent software. Comparison between numerical simulation and experimental results was analyzed to evaluate the effectiveness and accuracy of the numerical simulation, and to subsequently propose a simulation method to estimate the explosion hazard of a syngas/air mixture in a confined space.

Experimental apparatus and setup

The experimental apparatus consisted of a 6.91 L (diameter 20 cm, length 22 cm) constant volume combustion chamber (CVCC), flow controllers, a pressure transducer, a pressure transmitter and an ignition system, shown schematically in Fig. 1. A detailed description of the experimental facility can be found in a previous study by this group [12], therefore only